

APPLICATIONS OF INTEGRAL TRANSFORMS IN FRACTIONAL DIFFUSION PROCESSES

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The fundamental solution (Green function) for the Cauchy problem of the space-time fractional diffusion equation is investigated with respect to its scaling and similarity properties, starting from its Fourier-Laplace representation. Then, by using the Mellin transform, a general representation of the Green function in terms of Mellin-Barnes integrals in the complex plane is derived. This allows us to obtain a suitable computational form of the Green function in the space-time domain and to analyse its probability interpretation.

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1 INTRODUCTION

In this paper, we review the Cauchy problem for the *space-time fractional* partial differential equation, which is obtained from the standard diffusion equation by replacing the second-order space derivative with a Riesz-Feller derivative of order $\alpha \in (0, 2]$ and skewness θ ($|\theta| \leq \min\{\alpha, 2 - \alpha\}$), and the first-order time derivative with a Caputo derivative of order $\beta \in (0, 2]$.

The fundamental solution (Green function) for the Cauchy problem is investigated with respect to its scaling and similarity properties, starting from its Fourier-Laplace representation. In the cases $\{0 < \alpha \leq 2, \beta = 1\}$ and $\{\alpha = 2, 0 < \beta \leq 1\}$, the fundamental solution is known to be interpreted as a *spatial probability density function evolving in time*, so we talk of *space-fractional diffusion* and *time-fractional diffusion*, respectively. Then, by using the Mellin transform, we provide a general representation of the Green functions in terms of Mellin-Barnes integrals in the complex plane, which allows us *to extend the probability interpretation to the ranges* $\{0 < \alpha \leq 2, 0 < \beta \leq 1\}$ *and* $\{1 < \beta \leq \alpha \leq 2\}$.

Furthermore, from this representation it is possible to derive explicit formulae (convergent series and asymptotic expansions), which enable us to plot the spatial probability densities for different values of the relevant parameters α, θ, β .

2 THE GREEN FUNCTION

By replacing in the standard diffusion equation

$$\frac{\partial}{\partial t} u(x, t) = \frac{\partial^2}{\partial x^2} u(x, t), \quad -\infty < x < +\infty, \quad t \geq 0, \quad (1)$$

where $u = u(x, t)$ is the (real) field variable, the second-order space derivative and the first-order time derivative by suitable *integro-differential* operators, which can be interpreted as a space and time derivative of fractional order, we obtain a sort of "generalized diffusion" equation. Such equation may be referred to as the *space-time-fractional diffusion* equation when its fundamental solution (see below) can be interpreted as a probability density. We write

$${}_t D_*^\beta u(x, t) = {}_x D_\theta^\alpha u(x, t), \quad -\infty < x < +\infty, \quad t \geq 0, \quad (2)$$

where the α, θ, β are real parameters restricted as follows

$$0 < \alpha \leq 2, \quad |\theta| \leq \min\{\alpha, 2 - \alpha\}, \quad 0 < \beta \leq 2. \quad (3)$$

In Eq. (2) ${}_x D_\theta^\alpha$ is the space-fractional *Riesz-Feller derivative* of order α and skewness θ , and ${}_t D_*^\beta$ is the time-fractional *Caputo derivative* of order β . The definitions of these fractional derivatives are more easily understood if given in terms of Fourier transform and Laplace transform, respectively.

For the space-fractional *Riesz-Feller derivative* we have

$$\mathcal{F} \{ {}_x D_\theta^\alpha f(x); \kappa \} = -\psi_\alpha^\theta(\kappa) \widehat{f}(\kappa), \quad (4)$$

$$\psi_\alpha^\theta(\kappa) = |\kappa|^\alpha e^{i(\text{sign } \kappa)\theta\pi/2}, \quad \kappa \in \mathbb{R},$$

where $\widehat{f}(\kappa) = \mathcal{F} \{ f(x); \kappa \} = \int_{-\infty}^{+\infty} e^{i\kappa x} f(x) dx$. In other words the symbol of the pseudo-differential operator¹ ${}_x D_\theta^\alpha$ is required to be the logarithm of the characteristic function of the generic *stable* (in the Lévy sense) probability density, according to the Feller parameterization [1, 2], see also Refs. [3, 4]. For $\alpha = 2$ (hence $\theta = 0$) we have $\widehat{{}_x D_0^2}(\kappa) = -\kappa^2 = (-i\kappa)^2$, so we recover the standard second derivative. More generally for $\theta = 0$ we have $\widehat{{}_x D_0^\alpha}(\kappa) = -|\kappa|^\alpha = -(\kappa^2)^{\alpha/2}$ so

$${}_x D_0^\alpha = - \left(-\frac{d^2}{dx^2} \right)^{\alpha/2}. \quad (5)$$

In this case we call the LHS of Eq.(5) simply the *Riesz fractional derivative* operator of order α . Assuming $\alpha \neq 1, 2$ and taking θ in its range, one can show that the explicit expression of the *Riesz-Feller fractional derivative* obtained from Eq. (4) is

$${}_x D_\theta^\alpha f(x) := - [c_+(\alpha, \theta) {}_x D_+^\alpha + c_-(\alpha, \theta) {}_x D_-^\alpha] f(x), \quad (6)$$

where

$$c_+(\alpha, \theta) = \frac{\sin [(\alpha - \theta)\pi/2]}{\sin(\alpha\pi)}, \quad c_-(\alpha, \theta) = \frac{\sin [(\alpha + \theta)\pi/2]}{\sin(\alpha\pi)}, \quad (7)$$

and the ${}_x D_\pm^\alpha$ are Weyl fractional derivatives defined as

$${}_x D_\pm^\alpha f(x) = \begin{cases} \pm \frac{d}{dx} [{}_x I_\pm^{1-\alpha} f(x)] , & \text{if } 0 < \alpha < 1, \\ \frac{d^2}{dx^2} [{}_x I_\pm^{2-\alpha} f(x)] , & \text{if } 1 < \alpha < 2. \end{cases} \quad (8)$$

In Eq. (8) the ${}_x I_\pm^\mu$ ($\mu > 0$) denote the Weyl fractional integrals defined as

$$\begin{cases} {}_x I_+^\mu f(x) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^x (x - \xi)^{\mu-1} f(\xi) d\xi, \\ {}_x I_-^\mu f(x) = \frac{1}{\Gamma(\mu)} \int_x^{+\infty} (\xi - x)^{\mu-1} f(\xi) d\xi. \end{cases} \quad (\mu > 0) \quad (9)$$

¹ Let us recall that a generic linear pseudo-differential operator A , acting with respect to the variable $x \in \mathbb{R}$, is defined through its Fourier representation, namely $\int_{-\infty}^{+\infty} e^{i\kappa x} A[f(x)] dx = \widehat{A}(\kappa) \widehat{f}(\kappa)$, where $\widehat{A}(\kappa)$ is referred to as symbol of A , given as $\widehat{A}(\kappa) = (A e^{-i\kappa x}) e^{+i\kappa x}$.

In the particular case $\theta = 0$ we get $c_+(\alpha, 0) = c_-(\alpha, 0) = 1/[2 \cos(\alpha\pi/2)]$, and, by passing to the limit for $\alpha \rightarrow 2^-$, we get $c_+(2, 0) = c_-(2, 0) = -1/2$.

For $\alpha = 1$ we have

$${}_xD_\theta^1 f(x) = [\cos(\theta\pi/2) {}_xD_0^1 + \sin(\theta\pi/2) {}_xD] f(x), \quad (10)$$

with ${}_xD f(x) = \frac{d}{dx} f(x)$, and

$${}_xD_0^1 f(x) = -\frac{d}{dx} [{}_xH f(x)], \quad {}_xH f(x) = \frac{1}{\pi} \left(\int_{-\infty}^{+\infty} \frac{f(\xi)}{x - \xi} d\xi \right). \quad (11)$$

In (11) the operator ${}_xH$ denotes the Hilbert transform and its singular integral is understood in the Cauchy principal value sense.

The operator ${}_xD_\theta^\alpha$ has been referred to as the *Riesz-Feller* fractional derivative since both Marcel Riesz and William Feller contributed to its definition².

Let us now consider the time-fractional *Caputo derivative*. Following the original idea by Caputo [5], see also [6, 7, 8], a proper time fractional derivative of order $\beta \in (m-1, m]$ with $m \in \mathbb{N}$, useful for physical applications, may be defined in terms of the following rule for the Laplace transform

$$\mathcal{L} \{ {}_tD_*^\beta f(t); s \} = s^\beta \tilde{f}(s) - \sum_{k=0}^{m-1} s^{\beta-1-k} f^{(k)}(0^+), \quad m-1 < \beta \leq m. \quad (12)$$

where $\tilde{f}(s) = \mathcal{L} \{ f(t); s \} = \int_0^\infty e^{-st} f(t) dt$. Then the *Caputo fractional derivative* of $f(t)$ turns out to be defined as

$${}_tD_*^\beta f(t) := \begin{cases} \frac{1}{\Gamma(m-\beta)} \int_0^t \frac{f^{(m)}(\tau) d\tau}{(t-\tau)^{\beta+1-m}}, & m-1 < \beta < m, \\ \frac{d^m}{dt^m} f(t), & \beta = m. \end{cases} \quad (13)$$

In other words the operator ${}_tD_*^\beta$ is required to generalize the well-known rule for the Laplace transform of the n -th order derivative of a given (causal)

²Originally, in the late 1940's, Riesz [9] introduced the pseudo-differential operator ${}_xI_0^\alpha$ whose symbol is $|\kappa|^{-\alpha}$, well defined for any positive α with the exclusion of odd integer numbers, afterwards named the *Riesz potential*. The Riesz fractional derivative ${}_xD_0^\alpha := -{}_xI_0^{-\alpha}$ defined by analytical continuation was generalized by Feller in his 1952 genial paper [1] to include the skewness parameter of the strictly stable densities.

function keeping the standard initial value of the function itself and of its derivatives up to order $n - 1$ ³.

The fundamental solution (or the *Green function*) $G_{\alpha,\beta}^\theta(x, t)$ of Eq. (2) is the solution corresponding to the initial condition $u(x, 0^+) = \delta(x)$. We note that if $1 < \beta \leq 2$ we add the condition $u_t(x, 0^+) = 0$.

In the particular case of the standard diffusion equation (1) the Green function is nothing but the Gaussian probability density function with variance $\sigma^2 = 2t$, namely

$$G_{2,1}^0(x, t) = \frac{1}{2\sqrt{\pi}} t^{-1/2} e^{-x^2/(4t)}. \quad (14)$$

We note that in the limiting case $\{\alpha = \beta = 2\}$ we recover the D'Alembert *wave equation* with Green function $G_{2,2}^0(x, t) = [\delta(x + t) + \delta(x - t)]/2$.

In the general case the application of the transforms of Fourier and Laplace in succession to Eq (2) yields

$$-\psi_\alpha^\theta(\kappa) \widehat{G_{\alpha,\beta}^\theta}(\kappa, s) = s^\beta \widehat{G_{\alpha,\beta}^\theta}(\kappa, s) - s^{\beta-1}, \quad (15)$$

³ The reader should observe that the *Caputo* fractional derivative differs from the usual *Riemann-Liouville* fractional derivative which, defined as the left inverse of the Riemann-Liouville fractional integral, is here denoted as ${}_t D^\beta f(t)$. We have, see *e.g.* [11],

$${}_t D^\beta f(t) := \begin{cases} \frac{d^m}{dt^m} \left[\frac{1}{\Gamma(m-\beta)} \int_0^t \frac{f(\tau) d\tau}{(t-\tau)^{\beta+1-m}} \right], & m-1 \leq \beta < m, \\ \frac{d^m}{dt^m} f(t), & \beta = m. \end{cases}$$

When β is not integer and both fractional derivatives exist we have between them the following relation, see *e.g.* [7],

$${}_t D_*^\beta f(t) = {}_t D^\beta \left[f(t) - \sum_{k=0}^{m-1} f^{(k)}(0^+) \frac{t^k}{k!} \right], \quad m-1 < \beta < m,$$

or

$${}_t D_*^\beta f(t) = {}_t D^\beta f(t) - \sum_{k=0}^{m-1} f^{(k)}(0^+) \frac{t^{k-\beta}}{\Gamma(k-\beta+1)}, \quad m-1 < \beta < m.$$

The *Caputo* fractional derivative, originally ignored in the mathematical treatises, represents a sort of regularization in the time origin for the *Riemann-Liouville* fractional derivative and satisfies the relevant property of being zero when applied to a constant. For more details on this fractional derivative we refer the interested reader to Gorenflo and Mainardi [7] and Podlubny [8].

Added Note: Nowadays the reader can find an exhaustive treatment of fractional derivatives in the treatise by A.A. Kilbas, H.M. Srivastava and J.J. Trujillo, *Theory and Applications of Fractional Differential Equations*, Elsevier, Amsterdam (2006).

namely

$$\widehat{G_{\alpha,\beta}^\theta}(\kappa, s) = \frac{s^{\beta-1}}{s^\beta + \psi_\alpha^\theta(\kappa)}. \quad (16)$$

By using the known scaling rules for the Fourier and Laplace transforms, following the arguments by Mainardi *et al.* [10] one can prove without inverting Eq. (16) that $G_{\alpha,\beta}^\theta(x, t)$ has the scaling property

$$G_{\alpha,\beta}^\theta(x, t) = t^{-\beta/\alpha} K_{\alpha,\beta}^\theta(x/t^{\beta/\alpha}). \quad (17)$$

Here $x/t^{\beta/\alpha}$ acts as the similarity variable and $K_{\alpha,\beta}^\theta(\cdot)$ as the *reduced Green function*. For the analytical and computational determination of the reduced Green function we can restrict the attention to $x > 0$ because of the *symmetry relation* $K_{\alpha,\beta}^\theta(-x) = K_{\alpha,\beta}^\theta(x)$. Extending the paper by Gorenflo *et al.* [12] where the space-time fractional diffusion equation has been considered with the restriction $\{1 < \alpha \leq 2, \theta = 0, 0 < \beta \leq 2\}$, Mainardi *et al.* [10] have first inverted the Laplace transform and then have obtained the following Fourier integral representation of the reduced Green function

$$K_{\alpha,\beta}^\theta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\kappa x} E_\beta[-\psi_\alpha^\theta(\kappa)] d\kappa. \quad (18)$$

Here E_β denotes the entire transcendental function, known as the Mittag-Leffler function of order β , defined in the complex plane by the power series

$$E_\beta(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\beta n + 1)}, \quad \beta > 0, \quad z \in \mathcal{C}. \quad (19)$$

For detailed information on the Mittag-Leffler function the interested reader may consult *e.g.* [13] (Vol. 3, Ch. 18, pp. 206-227) and [7, 8, 11, 14]. By using the convolution theorem for the Mellin transform⁴, the authors in Ref.

⁴If

$$\mathcal{M}\{f(r); s\} = f^*(s) = \int_0^{+\infty} f(r) r^{s-1} dr, \quad \gamma_1 < \Re(s) < \gamma_2$$

denotes the Mellin transform of $f(r)$, the inversion is provided by

$$\mathcal{M}^{-1}\{f^*(s); r\} = f(r) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} f^*(s) r^{-s} ds$$

where $r > 0$, $\gamma = \Re(s)$, $\gamma_1 < \gamma < \gamma_2$. The Mellin convolution formula reads

$$h(r) = \int_0^\infty \frac{1}{\rho} f(\rho) g(r/\rho) d\rho \stackrel{\mathcal{M}}{\leftrightarrow} h^*(s) = f^*(s) g^*(s).$$

[10] have provided the Mellin-Barnes integral representation⁵ for the general case $0 < \alpha \leq 2$, $0 < \beta \leq 2$ as in Eqs. (2) and (3):

$$K_{\alpha,\beta}^{\theta}(x) = \frac{1}{\alpha x} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{\Gamma(\frac{s}{\alpha}) \Gamma(1 - \frac{s}{\alpha}) \Gamma(1-s)}{\Gamma(1 - \frac{\beta}{\alpha}s) \Gamma(\rho s) \Gamma(1 - \rho s)} x^s ds, \quad \rho = \frac{\alpha - \theta}{2\alpha}, \quad (20)$$

where $0 < \gamma < \min\{\alpha, 1\}$. Then, after changing s into $-s$ and using the known property $\Gamma(1+z) = z\Gamma(z)$, we can write the Mellin transform of $x K_{\alpha,\beta}^{\theta}(x)$ as

$$\int_0^{+\infty} K_{\alpha,\beta}^{\theta}(x) x^s dx = \rho \frac{\Gamma(1-s/\alpha) \Gamma(1+s/\alpha) \Gamma(1+s)}{\Gamma(1-\rho s) \Gamma(1+\rho s) \Gamma(1+\beta s/\alpha)}, \quad (21)$$

where $-\min\{\alpha, 1\} < \Re(s) < \alpha$. In particular we find $\int_0^{+\infty} K_{\alpha,\beta}^{\theta}(x) dx = \rho$ (with $\rho = 1/2$ if $\theta = 0$). We note that Eq. (21) is strictly valid as soon as cancellations in the "gamma fraction" at the RHS are not possible. Then this equation allows us to evaluate (in \mathbb{R}_0^+) the (absolute) moments of order δ for the Green function if $-\min\{\alpha, 1\} < \delta < \alpha$. In other words, it states that $K_{\alpha,\beta}^{\theta}(x) = \mathcal{O}(x^{-(\alpha+1)})$ as $x \rightarrow +\infty$. When cancellations occur in the "gamma fraction" the range of δ may change. An interesting case is $\{\alpha = 2, \theta = 0, 0 < \beta < 2\}$ (*time-fractional diffusion* including *standard diffusion*), where Eq. (21) reduces to

$$\int_0^{+\infty} K_{2,\beta}^0(x) x^s dx = \frac{1}{2} \frac{\Gamma(1+s)}{\Gamma(1+\beta s/2)}, \quad \Re(s) > -1. \quad (22)$$

This result proves the existence of all moments of order $\delta > -1$ for the corresponding Green function which reads

$$K_{2,\beta}^0(x) = \frac{1}{2} M_{\beta/2}(x) = \frac{1}{2x} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{\Gamma(1-s)}{\Gamma(1-\beta s/2)} x^s ds, \quad x > 0, \quad (23)$$

where $M_{\beta/2}$ denotes a function of the Wright type introduced by Mainardi [16, 17], see also [8, 18, 19]. For the case $\alpha = \beta$ (that we call *neutral-*

⁵ The names refer to the two authors, who in the beginning of the past century developed the theory of these integrals using them for a complete integration of the hypergeometric differential equation. However, as pointed out in [13] (Vol. 1, Ch. 1, §1.19, p. 49), these integrals were first used by S. Pincherle in 1888. For a revisited analysis of the pioneering work of Pincherle (Professor of Mathematics at the University of Bologna from 1880 to 1928) we refer to the recent paper by Mainardi and Pagnini [15]. As a matter of fact this type of integrals turns out to be useful in inverting the Mellin transform.

fractional diffusion) we obtain from (20) an elementary expression

$$\begin{aligned}
K_{\alpha,\alpha}^{\theta}(x) &= N_{\alpha}^{\theta}(x) = \frac{1}{\alpha x} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{\Gamma(\frac{s}{\alpha}) \Gamma(1 - \frac{s}{\alpha})}{\Gamma(\rho s) \Gamma(1 - \rho s)} x^s ds \\
&= \frac{1}{\alpha x} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{\sin(\pi \rho s)}{\sin(\pi s/\alpha)} x^s ds = \frac{1}{\pi} \frac{x^{\alpha-1} \sin[\frac{\pi}{2}(\alpha - \theta)]}{1 + 2x^{\alpha} \cos[\frac{\pi}{2}(\alpha - \theta)] + x^{2\alpha}}.
\end{aligned} \tag{24}$$

where $0 < \gamma < \alpha$.

We note that the Mellin-Barnes integral representation allows us to construct computationally the fundamental solutions of Eq. (2) for any triplet $\{\alpha, \beta, \theta\}$ ($\alpha \neq \beta$) by matching their convergent and asymptotic expansions, as shown in [10]. Readers acquainted with Fox H functions can recognize in Eq. (20) the representation of a certain function of this class, see *e.g.* [4, 11, 20, 21]. Unfortunately, as far as we know, computing routines for this general class of special functions are not yet available⁶.

Let us now point out that, in the peculiar cases of *space-fractional-diffusion*, *time-fractional-diffusion*, and *neutral-fractional-diffusion*, non-negativity of the corresponding Green functions can be proven; being normalized in \mathbb{R} these functions can indeed be interpreted as probability densities. In particular, for $\beta = 1$ and $0 < \alpha < 2$ (*strictly space-fractional diffusion*) we recover the class of the strictly stable (non-Gaussian) densities $L_{\alpha}^{\theta}(x)$ exhibiting fat tails (with the algebraic decay $\propto |x|^{-(\alpha+1)}$) and infinite variance, whereas for $\alpha = 2$ and $0 < \beta < 1$ (*strictly time-fractional diffusion*) the class of the Wright-type densities $M_{\beta/2}(x)/2$ exhibiting stretched exponential tails and finite variance proportional to t^{β} .

The meaning of probability density can be extended under proper conditions to the reduced Green function of the *space-time-fractional* partial differential equation (2) in virtue of the following identity, proven in Ref. [10],

$$K_{\alpha,\beta}^{\theta}(x) = \begin{cases} \alpha \int_0^{\infty} [\xi^{\alpha-1} M_{\beta}(\xi^{\alpha})] L_{\alpha}^{\theta}(x/\xi) \frac{d\xi}{\xi}, & 0 < \beta < 1, \\ \int_0^{\infty} M_{\beta/\alpha}(\xi) N_{\alpha}^{\theta}(x/\xi) \frac{d\xi}{\xi}, & 0 < \beta/\alpha < 1. \end{cases} \tag{25}$$

Then, due to the previous discussion, in the cases $\{0 < \alpha < 2, 0 < \beta < 1\}$ and $\{1 < \beta \leq \alpha < 2\}$ we obtain a class of probability densities (symmetric or

⁶ *Added Note* Nowadays the reader can find the representation of the fundamental solutions in terms of Fox H functions in the paper by F. Mainardi, G. Pagnini and R.K. Saxena, Fox H functions in fractional diffusion, *J. Computational and Applied Mathematics* **178**, 321-331 (2005).

non-symmetric according to $\theta = 0$ or $\theta \neq 0$) which exhibit fat tails with an algebraic decay $\propto |x|^{-(\alpha+1)}$. Thus, they belong to the domain of attraction of the Lévy stable densities of index α and can be referred to as *fractional stable densities*.

3 CONCLUSIONS

The above analysis of the Cauchy problem for the *space-time fractional* diffusion equation shows the fundamental and combined roles of the integral transforms of Fourier, Laplace and Mellin type. By the aid of the transforms of Fourier and Laplace the scaling and similarity properties of the Green function can be easily derived. The Mellin transform allows us to obtain for the Green function a general representation in terms of Mellin-Barnes integrals (hence a computational form in terms of convergent and asymptotic series), and the extension of its probability interpretation⁷

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⁷*Added Note* It is worthwhile to attract the reader's attention to the role of the Mellin transform to derive subordination laws in fractional diffusion processes, see F. Mainardi, G. Pagnini and R. Gorenflo, Mellin transform and subordination laws in fractional diffusion processes, *Fractional Calculus and Applied Analysis* **6** No. 4, 441-459 (2003). [E-print <http://arxiv.org/abs/math/0702133>]

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